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The Noble-Abel Equation of State: Thermodynamic Derivations for Ballistics Modelling

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ABSTRACT

Accurate modelling of gun interior ballistics promotes more efficient gun and propelling charge design. In order to simulate interior ballistic flowfields, such models require a description of the thermodynamic behaviour of the propellant gas. The Noble-Abel equation provides a simple and reasonably accurate equation of state for propellant gases at the high densities and temperatures experienced in guns. Most computational fluid dynamics-based ballistics models, however, require additional thermodynamic functions which must be derived from the equation of state. This note presents the derivation of such thermodynamic functions for Noble-Abel gases. Although the derivations are geared toward the functional requirements of the commercial *Fluent* code, the results are equally applicable to all computational fluid dynamics solvers. Also presented is a brief numerical example for a typical propellant, highlighting the different thermodynamics of the Noble-Abel and ideal gas equations.

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EXECUTIVE SUMMARY

Accurate modelling of gun interior ballistics promotes more efficient gun and propelling charge design. In order to simulate interior ballistic flowfields, such models require a description of the thermodynamic behaviour of the propellant gas. The Noble-Abel equation provides a simple and reasonably accurate equation-of-state for propellant gases at the high densities and temperatures experienced in guns.

Most computational fluid dynamics-based ballistics models, however, require additional thermodynamic functions which must be derived from the equation-of-state. This note presents the derivation of a range of thermodynamic functions for Noble-Abel gases. They include:

- Entropy,
- Speed of sound,
- The functional form of the specific heats,
- The relationship between the specific heats and gas constant,
- The isentropic process, and
- Various partial derivatives of density and enthalpy.

Although the derivations are geared toward the functional requirements of the commercial *Fluent* code, the results are equally applicable to all computational fluid dynamics solvers.

Also presented is a brief numerical example for a high-energy tank gun propellant (JA2), demonstrating the difference between the Noble-Abel and ideal gas equations-of-state and two of the derived functions.

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Nomenclature

a	Speed of Sound [m/s]
b	Co-volume [m ³ /kg]
c_p	Specific Heat at Constant Pressure [J/(kg K)]
c_v	Specific Heat at Constant Volume [J/(kg K)]
E	Intensive Total Energy [J/kg]
e	Internal Energy [J/kg]
\mathbf{F}	Vector of Fluxes
h	Enthalpy [J/kg]
$\hat{\mathbf{n}}$	Normal Unit Vector
P	Pressure [Pa]
R	Specific Gas Constant [J/(kg K)]
s	Entropy [J/(kg K)]
S	Surface Area [m ²]
t	Time [s]
T	Temperature [K]
\mathbf{u}	Velocity Vector [m/s]
\mathbf{U}	Vector of Conserved Variables
v	Specific Volume [m ³ /kg]
V	Volume [m ³]
α	Coefficient for Intermolecular Attraction [m ⁵ /(kg s ²)]
γ	Ratio of Specific Heats
ρ	Density [kg/m ³]

1 Introduction

The capability to accurately model gun interior ballistics (IB) promotes faster and cheaper gun and propelling charge design. Likewise, modelling can be used to predict and assess a gun's performance characteristics before it is built, tested, purchased or modified. Although such a predictive utility can be partially achieved through targeted experiments, models provide a range of additional benefits. The extreme interior ballistic environment makes experimental instrumentation and measurement difficult, whereas it is normally possible to determine all modelled physical quantities throughout a simulation domain. The ability to add or remove different physical phenomena at will, allows models to be used to identify the relative action of the various ballistic processes. Modelling also allows automated optimization. For example, charge weight can be minimized by optimizing propellant grain geometry subject to muzzle velocity and maximum pressure constraints.

One of the simplest classes of IB models are lumped parameter models, such as IB-HVG2 [1], where the dynamic firing process is represented by mean (lumped) state variables. A particular pressure gradient between breech and projectile base is assumed and applied to calculate projectile base pressure and its resulting acceleration. Two-phase, multi-dimensional computational fluid dynamics flow (CFD) solvers, such as the NGEN [2] code, provide higher-fidelity IB simulations but are computationally expensive. Physical phenomena such as inter-phase drag, axial and radial flame spreading within the propellant bed, boundary layer formation, and pressure waves can be modelled using this class of tools. Of intermediate complexity are codes such as XKTC [3], which combines a one-dimensional flow solver with a lumped-parameter model.

Irrespective of which approach is used, all models require an accurate description of the thermodynamics of the propellant gas. Consider the Euler equations, which may be thought of as a simplified version of the Reynolds-averaged Navier-Stokes equations that are used by the CFD solvers to describe the ballistic flow. Assuming no source terms, for a control volume V the Euler equations can be written in integral form as

$$\frac{\partial}{\partial t} \int_V \mathbf{U} dV + \int_S \mathbf{F} dS = \mathbf{0}, \quad (1)$$

where \mathbf{U} is a vector representing conserved flow quantities at points within the control volume, \mathbf{F} is a vector of fluxes across the surface of the control volume, the scalars V and S refer to the volume and surface of the control volume respectively, and t is the time variable. For a single-species, single-phase flow, the vectors \mathbf{U} and \mathbf{F} may be expressed as

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \\ \rho E \end{bmatrix}, \quad \text{and} \quad \mathbf{F} = \begin{bmatrix} \rho(\mathbf{u} \cdot \hat{\mathbf{n}}) \\ \rho \mathbf{u}(\mathbf{u} \cdot \hat{\mathbf{n}}) + P \hat{\mathbf{n}} \\ \rho E(\mathbf{u} \cdot \hat{\mathbf{n}}) + P(\mathbf{u} \cdot \hat{\mathbf{n}}) \end{bmatrix}. \quad (2)$$

Here, \mathbf{u} is the fluid velocity vector and $\hat{\mathbf{n}}$ is a unit normal to the control volume surface. The primitive variables ρ , P , and E represent density, absolute static pressure, and intensive total energy respectively. Total energy can be expressed in terms of internal energy and kinetic energy as

$$E = e + \frac{1}{2} |\mathbf{u}|^2, \quad (3)$$

and internal energy can be calculated by integrating the constant-volume specific heat with respect to temperature:

$$e = \int_{T_{ref}}^T c_v dT. \quad (4)$$

Equations 1–4 contain six variables but provide only five relations. To solve the system an additional equation—relating the state variables of the fluid—must be provided.

For gases at moderate to low density, the ideal gas equation of state

$$P = \rho RT, \quad (5)$$

where R is the specific gas constant, can be used to close the system. The ideal gas equation of state is accurate providing that (1) the average intermolecular spacing or mean free path of the gas is very large compared to the size of the gas molecules, and (2) intermolecular forces are weak. For many practical flow regimes both of these assumptions are true. However, the high gas densities occurring in a gun chamber during combustion render the ideal gas equation of state inaccurate. Solid loading densities for gun propelling charges are typically of the order 500–1 000 kg/m³. Peak gas densities produced during the ballistic cycle may also approach this magnitude since, in most guns, the bulk of propellant is burnt before the projectile has moved very far downbore.

While still an approximation, the van der Waals equation of state provides an improvement in accuracy for high density gases. It is of the form [4]

$$(P + \alpha/v^2)(v - b) = RT, \quad (6)$$

where the gas specific volume $v \equiv 1/\rho$. The co-volume b compensates for the finite volume occupied by the gas molecules, while the term α/v^2 accounts for intermolecular attraction forces. Note that in the case $\alpha = b = 0$, Equation 6 reverts to the ideal gas equation of state. In ballistics applications, the high propellant gas temperature means that intermolecular attraction energy is small in comparison to molecular kinetic energy [4]. Thus the attraction term can be removed without significant loss of accuracy, resulting in the so-called Noble-Abel equation of state:

$$P(v - b) = RT. \quad (7)$$

Equation 7 can be used to describe the propellant gas with sufficient accuracy for both lumped parameter and CFD IB models. For lumped parameter modelling, nothing further is required. Most CFD models, however, require a range of additional thermodynamic functions corresponding to this equation of state. It is necessary to calculate sound speed, for example, in order to evaluate the Courant-Friedrich-Lewy criterion and maintain numerical stability; the expression for speed of sound in an ideal gas is different to that for Noble-Abel gases. Similarly, partial derivatives of state variables may be required quantities for certain implicit CFD schemes. The commercial *Fluent* CFD code [5], for example, requires eight thermodynamic functions that must be derived from (or are related to) the equation of state. The aim of this note is to present the derivation of such thermodynamic functions for a Noble-Abel gas. Although this note closely follows the requirements of the *Fluent* code, the results are equally applicable to all commercial and research CFD solvers. Also presented is a numerical example for a typical propellant, comparing thermodynamic quantities calculated under the Noble-Abel equation of state with those of an ideal gas.

2 Thermodynamic Functions

The *Fluent* code requires definitions for the thermodynamic functions listed below [5]. These functions, and some additional relations, are derived in Sections 2.1–2.7.

$$\begin{array}{ccccccc} \rho(T, P) & c_p(T, \rho) & h(T, \rho) & s(T, \rho) & a(T, \rho) & & \\ \left(\frac{\partial \rho}{\partial T}\right)_P & \left(\frac{\partial \rho}{\partial P}\right)_T & \left(\frac{\partial h}{\partial T}\right)_P & \left(\frac{\partial h}{\partial P}\right)_T & & & \end{array}$$

2.1 Equation of State

The Noble-Abel equation of state has already been defined in the introduction as

$$P(v - b) = RT,$$

however *Fluent* requires an equation of state in the form $\rho(T, P)$. It is easy to recast the equation as

$$\rho = P / (RT + bP) \quad (8)$$

to satisfy this requirement.

2.2 Specific Heats

Fluent also requires the specific heat at constant pressure as a function of density and temperature. For completeness we will consider both specific heats in this subsection. They are defined as

$$c_p \equiv \left(\frac{\partial h}{\partial T}\right)_p \quad \text{and} \quad c_v \equiv \left(\frac{\partial e}{\partial T}\right)_v. \quad (9)$$

From Reference [6], the gradient of c_p with respect to pressure at constant temperature can be related to the equation of state via

$$\left(\frac{\partial c_p}{\partial P}\right)_T = -T \left(\frac{\partial^2 v}{\partial T^2}\right)_P. \quad (10)$$

Evaluating the right hand side for the Noble-Abel equation of state yields

$$\left(\frac{\partial c_p}{\partial P}\right)_T = -T \frac{\partial^2}{\partial T^2} \left(\frac{RT}{P} + b\right)_P = 0. \quad (11)$$

By Equation 8 this also proves that $(\partial c_p / \partial \rho)_T = 0$, and hence

$$c_p(\rho, T) = c_p(T) \quad (12)$$

for a Noble-Abel gas. A similar proof is possible for specific heat at constant volume:

$$\left(\frac{\partial c_v}{\partial v}\right)_T = T \left(\frac{\partial^2 P}{\partial T^2}\right)_v = T \frac{\partial^2}{\partial T^2} \left(\frac{RT}{v - b}\right)_v = 0, \quad (13)$$

and thus

$$c_v(\rho, T) = c_v(T). \quad (14)$$

Results 12 and 14 show that, for a Noble-Abel gas, the specific heat functions can be conveniently implemented in computer code as a curve fit or look-up table in terms of temperature only. As an alternative to providing the specific heats as a function of temperature, the calorifically perfect approximation could also be made:

$$c_p = \text{constant} \quad \text{and} \quad c_v = \text{constant}. \quad (15)$$

2.3 The Specific Gas Constant

The previous section showed that both c_p and c_v could be expressed as functions of temperature only. We now proceed to show that these quantities can be related, such that if one specific heat is known then the other may be calculated easily. This obviates the need to provide two separate tables (or curve fits). From Reference [6]

$$c_p - c_v = -T \left(\frac{\partial v}{\partial T} \right)_P^2 \left(\frac{\partial P}{\partial v} \right)_T \quad (16)$$

Evaluating the partial derivatives from the Noble-Abel equation of state yields

$$c_p - c_v = T \left(\frac{R}{P} \right)^2 \frac{RT}{(v - b)^2}. \quad (17)$$

Upon simplifying, we get the convenient relationship

$$c_p - c_v = R, \quad (18)$$

which is the same as that for ideal gases.

2.4 Entropy

Entropy for a Noble-Abel gas may be derived starting from the thermodynamic relation

$$Tds = de + PdV. \quad (19)$$

Substituting with Equations 7 and 9, we have

$$ds = c_v \frac{dT}{T} + \frac{R}{v - b} dv. \quad (20)$$

Equation 20 may be integrated to calculate the entropy difference between two states:

$$s_2 - s_1 = \int_{T_1}^{T_2} \frac{c_v}{T} dT + \int_{v_1}^{v_2} \frac{R}{v - b} dv. \quad (21)$$

The second term is easy to evaluate, however the first term can only be analytically integrated if the form of c_v is known. For the case of a calorifically perfect gas (Equation 15), integration yields

$$s_2 - s_1 = c_v \ln \left(\frac{T_2}{T_1} \right) + R \ln \left(\frac{v_2 - b}{v_1 - b} \right), \quad (22)$$

or equivalently, in the form required by *Fluent*,

$$s_2 - s_1 = c_v \ln \left(\frac{T_2}{T_1} \right) + R \ln \left(\frac{1/\rho_2 - b}{1/\rho_1 - b} \right). \quad (23)$$

2.5 The Isentropic Process

Although not directly important to ballistics modelling, the consideration of state changes occurring at constant entropy yields a result that will be of use in the following section. For an isentropic process $s_1 = s_2$, and for a calorifically perfect gas Equation 22 gives

$$\ln \left(\frac{T_2}{T_1} \right) = -\frac{R}{c_v} \ln \left(\frac{v_2 - b}{v_1 - b} \right) \quad (24)$$

and thus

$$\frac{T_2}{T_1} = \left(\frac{v_1 - b}{v_2 - b} \right)^{R/c_v}. \quad (25)$$

Replacing the temperature terms by pressure and specific volume (Equation 7) yields

$$\frac{P_2(v_2 - b)}{P_1(v_1 - b)} = \left(\frac{v_1 - b}{v_2 - b} \right)^{R/c_v}, \quad (26)$$

and

$$P_1(v_1 - b)^{(1+R/c_v)} = P_2(v_2 - b)^{(1+R/c_v)}. \quad (27)$$

The ratio of specific heats is defined as $\gamma \equiv c_p/c_v$, which together with Equation 18 results in the expression

$$P(v - b)^\gamma = \text{constant} \quad (28)$$

for an isentropic process in a calorifically perfect, Noble-Abel gas. This is analagous to the familiar ideal-gas expression $Pv^\gamma = \text{constant}$.

2.6 Sound Speed

The speed of sound in a gas, a , is defined as the speed of reversible pressure wave propagation. From Reference [7], this is

$$a = \left(\frac{\partial P}{\partial \rho} \right)_s^{1/2}. \quad (29)$$

We may expand the partial derivative using the chain rule

$$\left(\frac{\partial P}{\partial \rho} \right)_s = \left(\frac{\partial P}{\partial v} \frac{\partial v}{\partial \rho} \right)_s, \quad (30)$$

and since specific volume is just the reciprocal of density

$$\left(\frac{\partial P}{\partial \rho}\right)_s = -\left(\frac{\partial P}{\partial v}\right)_s v^2. \quad (31)$$

We now take the partial derivative of both sides of Equation 28 with respect to specific volume

$$\frac{\partial}{\partial v}[P(v-b)^\gamma] = 0, \quad (32)$$

and by the product rule

$$\frac{\partial P}{\partial v}(v-b)^\gamma + P\gamma(v-b)^{(\gamma-1)} = 0. \quad (33)$$

Remembering that Equation 28 represented an isentropic process in a calorifically perfect gas, we therefore have

$$\left(\frac{\partial P}{\partial v}\right)_s = -\frac{P\gamma}{v-b}. \quad (34)$$

Finally, substitution of Equations 34 and 7 into Equation 31 yields the speed of sound in a calorifically perfect Noble-Abel gas:

$$a = \frac{v}{v-b} \sqrt{\gamma RT}. \quad (35)$$

This expression may be thought of as the speed of sound in an ideal gas, $\sqrt{\gamma RT}$, with a premultiplying coefficient to correct for the effect of co-volume. It is easily rewritten in the form required by *Fluent*,

$$a = \frac{1}{1-b\rho} \sqrt{\gamma RT}. \quad (36)$$

It can be shown that Equation 36 also holds for the more general case of Noble-Abel gases which are not calorifically perfect. In Reference [7], Anderson derives the general expression

$$a^2 = \frac{\gamma P}{\rho} \left[\frac{1 + (1/P)(\partial e / \partial v)_T}{1 - \rho(\partial h / \partial P)_T} \right] \quad (37)$$

for the sound speed of non-ideal gases, reacting gases, and thermally and calorifically imperfect gases. The partial derivatives of Equation 37 can be evaluated using two thermodynamic relations given in [6]. The partial derivative of internal energy with respect to specific volume at constant temperature can be related to the equation of state via

$$\left(\frac{\partial e}{\partial v}\right)_T = T \left(\frac{\partial P}{\partial T}\right)_v - P. \quad (38)$$

Upon substitution of Equation 7, we have

$$\left(\frac{\partial e}{\partial v}\right)_T = \frac{RT}{v-b} - P = 0. \quad (39)$$

Likewise, the partial derivative of enthalpy with respect to pressure at constant temperature can be evaluated by the relation

$$\left(\frac{\partial h}{\partial P}\right)_T = v - T \left(\frac{\partial v}{\partial T}\right)_P. \quad (40)$$

For the Noble-Abel equation of state, this yields

$$\left(\frac{\partial h}{\partial P}\right)_T = v - \frac{RT}{P} = b. \quad (41)$$

After substitution of Equations 41 and 39 into Equation 37 we have

$$a^2 = \frac{\gamma P}{\rho} \left[\frac{1}{1 - b\rho} \right], \quad (42)$$

which can be simplified to give

$$a = \frac{1}{1 - b\rho} \sqrt{\gamma RT}. \quad (43)$$

This expression is identical to the sound speed for calorifically perfect Noble-Abel gases given by Equation 36.

2.7 Partial Derivatives of State Variables

The *Fluent* code additionally requires that various partial derivatives of state variables be supplied. Derivations of the non-trivial partial derivatives are now provided.

First we derive the partial derivative of density with respect to pressure at constant temperature, starting with the chain rule

$$\left(\frac{\partial \rho}{\partial P}\right)_T = \left(\frac{\partial \rho}{\partial v} \frac{\partial v}{\partial P}\right)_T, \quad (44)$$

and thus

$$\left(\frac{\partial \rho}{\partial P}\right)_T = -\frac{1}{v^2} \left(\frac{\partial v}{\partial P}\right)_T. \quad (45)$$

From the Noble-Abel equation of state

$$\frac{\partial}{\partial P}(v - b)_T = \frac{\partial}{\partial P} \left(\frac{RT}{P} \right)_T, \quad (46)$$

so

$$\left(\frac{\partial v}{\partial P}\right)_T = -\frac{RT}{P^2}. \quad (47)$$

Substituting this into Equation 45 and simplifying yields the result

$$\left(\frac{\partial \rho}{\partial P}\right)_T = \frac{1}{RT} \left(\frac{v - b}{v} \right)^2, \quad (48)$$

which can be rewritten in the required form as

$$\left(\frac{\partial \rho}{\partial P}\right)_T = \frac{(1 - \rho b)^2}{RT}. \quad (49)$$

Fluent also needs the partial derivative of density with respect to temperature at constant pressure. A derivation similar to the above gives

$$\left(\frac{\partial \rho}{\partial T}\right)_P = \frac{b\rho^2 - \rho}{T}. \quad (50)$$

Finally, two partial derivatives of enthalpy are required by *Fluent*. The first, $(\partial h / \partial T)_P$ is by definition equal to c_p (Equation 9). The second, $(\partial h / \partial P)_T$ is equal to the co-volume b (Equation 41).

3 Example

A brief example is now presented, to demonstrate the difference between the Noble-Abel and ideal gas equations of state and two of the derived functions. A high performance tank gun propellant, JA2, will be used as the subject. The approximate thermodynamic properties of JA2 propellant gas, including its specific heats at the propellant flame temperature, are shown in Table 1.

Figure 1 shows pressure as a function of density and temperature for JA2 propellant gas, according to the Noble-Abel equation of state. The variation between pressure calculated using the Noble-Abel and ideal gas equations is represented by the coloured contours. At a typical IB gas density of 300 kg/m³, for example, the pressure difference is 30%. The differences in pressure are observed to be independent of temperature. This is to be expected, since the ideal and Noble-Abel equations of state can be related by a substitution in terms of specific volume (or density) only: $v \leftrightarrow (v - b)$.

Figure 2 shows sound speed as a function of density and temperature for JA2 propellant gas, assuming that it is calorifically perfect and obeys the Noble-Abel equation of state (Equation 35). Again, the difference between the Noble-Abel and ideal-gas values are represented by coloured contours and depend on density only. The differences are of similar magnitude to those already observed for pressure.

Entropy, as a function of density and temperature, is shown in Figure 3 for the Noble-Abel equation of state. The gas is assumed calorifically perfect. A reference entropy (s_1 in Equation 22) corresponding to a state of 300 K and 1 kg/m³ has been used. The difference between the Noble-Abel and ideal-gas entropy is shown in the figure in terms of absolute entropy values.

The effect of the equation of state on predicted ballistic performance is dependent on the particular gun and propellant properties, and the operating regime. In the case of JA2 propellant, muzzle velocity predictions for typical high performance medium-calibre guns can be expected to differ by around 10–15%. Likewise, peak gun chamber pressure predictions will be significantly higher (around 30–35%) when the Noble-Abel equation is used instead of the ideal gas equation. This is consistent with the results of Figure 1.

Table 1: Properties of JA2 Propellant Gas

Gas Constant, R	334 J/(kg K)
Specific Heat Ratio, γ	1.225
Specific Heat at Constant Volume, $c_v(T_f)$	1484 J/(kg K)
Specific Heat at Constant Pressure, $c_p(T_f)$	1818 J/(kg K)
Co-volume, b	0.001 m ³ /kg
Flame Temperature of Solid Propellant, T_f	3410 K

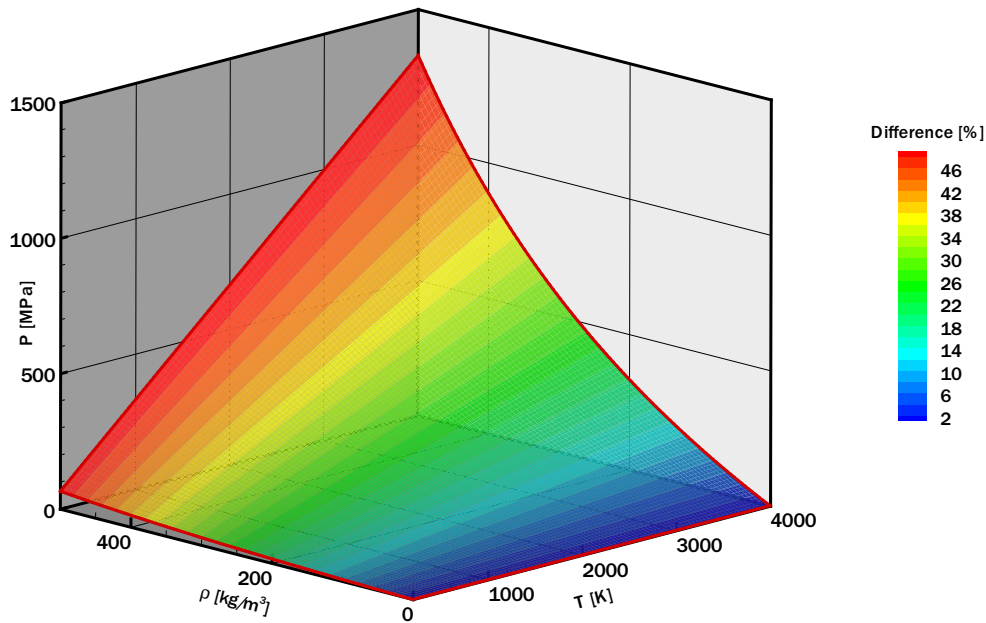


Figure 1: Pressure as a function of density and temperature for JA2 propellant gas, according to the Noble-Abel equation of state. Coloured contours indicate the difference between ideal gas and Noble-Abel gas results.

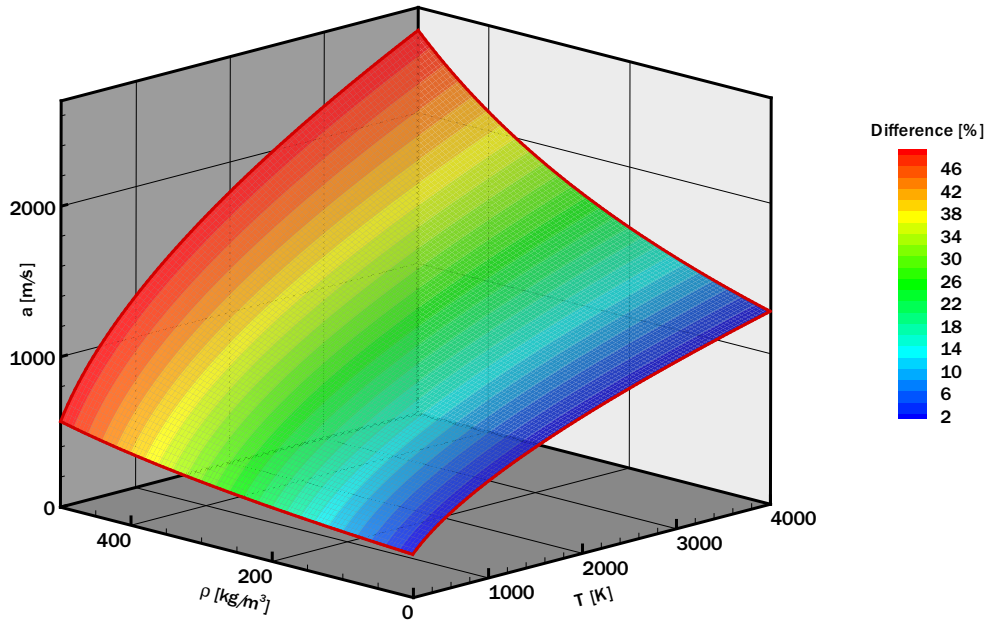


Figure 2: Sound speed as a function of density and temperature for JA2 propellant gas, according to the Noble-Abel equation of state. Coloured contours indicate the difference between ideal gas and Noble-Abel gas results.

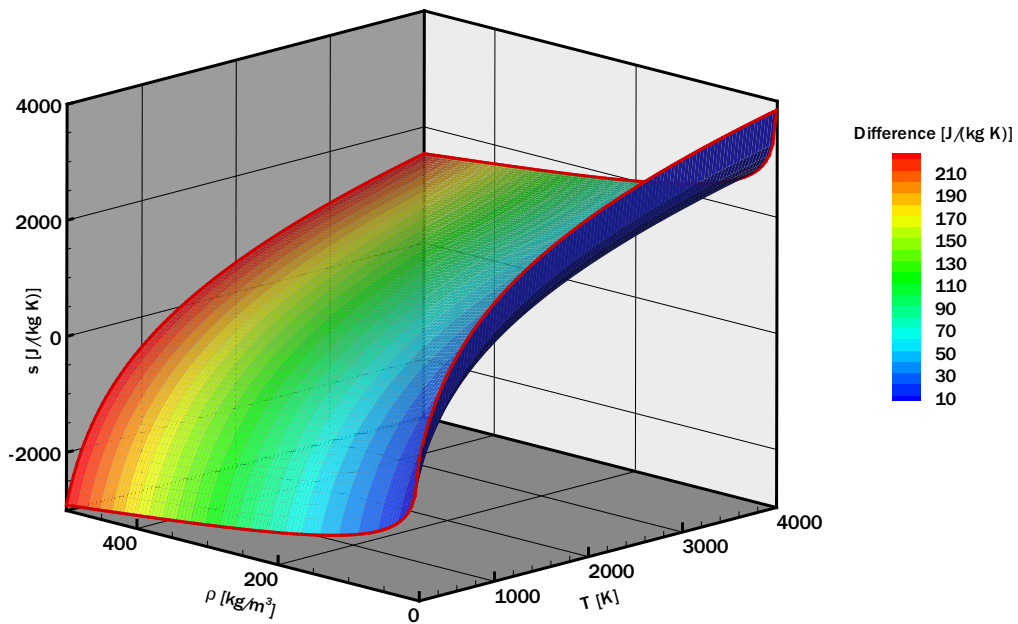


Figure 3: Entropy as a function of density and temperature for JA2 propellant gas, according to the Noble-Abel equation of state. Coloured contours indicate the difference between ideal gas and Noble-Abel gas calculations.

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19. ABSTRACT Accurate modelling of gun interior ballistics promotes more efficient gun and propelling charge design. In order to simulate interior ballistic flowfields, such models require a description of the thermodynamic behaviour of the propellant gas. The Noble-Abel equation provides a simple and reasonably accurate equation of state for propellant gases at the high densities and temperatures experienced in guns. Most computational fluid dynamics-based ballistics models, however, require additional thermodynamic functions which must be derived from the equation of state. This note presents the derivation of such thermodynamic functions for Noble-Abel gases. Although the derivations are geared toward the functional requirements of the commercial <i>Fluent</i> code, the results are equally applicable to all computational fluid dynamics solvers. Also presented is a brief numerical example for a typical propellant, highlighting the different thermodynamics of the Noble-Abel and ideal gas equations.					

